

Two-qubit mixed states more entangled than pure states: Comparison of the relative entropy of entanglement for a given nonlocality

Bohdan Horst,¹ Karol Bartkiewicz,^{2,*} and Adam Miranowicz¹

¹*Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland*

²*RCPTM, Joint Laboratory of Optics of Palacký University and Institute of Physics of Academy of Sciences of the Czech Republic, 17. listopadu 12, 772 07 Olomouc, Czech Republic*

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Amplitude damping changes entangled pure states into usually less-entangled mixed states. We show, however, that even local amplitude damping of one or two qubits can result in mixed states more entangled than pure states if one compares the relative entropy of entanglement (REE) for a given degree of the Bell-CHSH inequality violation (referred to as nonlocality). By applying Monte-Carlo simulations, we find the maximally-entangled mixed states and show that they are likely to be optimal by checking the Karush-Kuhn-Tucker conditions, which generalize the method of Lagrange multipliers for this nonlinear optimization problem. We show that the REE for mixed states can exceed that of pure states if the nonlocality is in the range (0,0.82) and the maximal difference between these REEs is 0.4. A former comparison [Phys. Rev. A **78**, 052308 (2008)] of the REE for a given negativity showed analogous property but the corresponding maximal difference in the REEs is one-order smaller (i.e., 0.039) and the negativity range is (0,0.53) only. For appropriate comparison, we normalized the nonlocality measure to be equal to the standard entanglement measures, including the negativity, for arbitrary two-qubit pure states. We also analyze the influence of the phase-damping channels on the entanglement of the initially pure states. We show that the minimum of the REE for a given nonlocality can be achieved by these two channels, contrary to the amplitude damping channel.

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I. INTRODUCTION

Quantum entanglement and nonlocality [1, 2] are among the central concepts in quantum theory providing powerful resources for modern quantum-information processing [3]. Nevertheless, despite of much progress (as reviewed in, e.g., Ref. [4]), our understanding of the relation between entanglement and nonlocality is very incomplete.

Quantum nonlocality is often discussed in the context of Bell's theorem, which can be, arguably, considered „the most profound discovery of science” [5]. The Bell inequality violation (BIV) for a given state implies that there is no physical theory of local-hidden variables which can reproduce the predictions for the state [1]. Although the BIV does not necessarily imply nonlocality and vice versa (see, e.g., Ref. [6]), for convenience, we use the terms BIV and nonlocality interchangeably.

Because of the prominent role of quantum entanglement, much effort has been devoted to investigating measures of entanglement that can be used for its quantification. Currently, a variety of formal and operational entanglement measures can be applied [4] depending on the physical and information contexts. For example, if one is interested in distinguishing entangled from separable states, a convenient choice is the relative entropy of entanglement (REE) [7]. However, if one considers the cost of entanglement under operations preserving the positivity of partial transpose (PPT) [8], the appropriate choice of entanglement measure is the (logarithmic) negativity [9, 10]. The concurrence [11] is yet another popular measure of entanglement, which quantifies the entanglement of formation [12].

In the case of two-qubit pure states some of the entanglement measures are equivalent (e.g., the negativity, concurrence and nonlocality). However, the situation is quite different for mixed states, where the states of the same value of a given entanglement measure can correspond to different values of entanglement quantified by other measures. Thus, it can happen that entangled states ordered according to one entanglement measure can be ordered differently by another measure [13–16].

The most interesting entangled states are, arguably, the boundary states, which are extremal in one measure for a given value of another measure. They can serve as “way-marks” for entangled states providing means for their systematic classification. Moreover, it turns out that some of the most entangled states according to the REE for a given value of another entanglement measure as, e.g., the negativity [17], are mixed states.

Some comparative studies of the nonlocality in relation to entanglement measures in a dynamical context of two qubits can be found in, e.g., Refs. [14, 18–20].

In this paper, we find maximally entangled mixed states (MEMS) corresponding to the largest REE for a given degree of nonlocality using the Horodecki measure [21, 22]. We also show that these MEMS are more entangled than pure states for a wide range of this nonlocality degree. As an indicator of extremality of the found MEMS we use the Karush-Kuhn-Tucker (KKT) conditions in a refined method of Lagrange multipliers.

The paper is organized as follows. In Sec. II, we introduce some basic definitions of the nonlocality and entanglement measures used in our paper. In Sec. III, we demonstrate analytically that there are mixed states more entangled than pure states when analyzing the REE for a fixed nonlocality

* bartkiewicz@jointlab.upol.cz

(and negativity). In Sec. IV, we describe how to physically obtain an important class of entangled states, which, as we show in Sec. V, are the boundary states if quantified by the REE for given values of the nonlocality, negativity, and concurrence. The most important result in this paper is finding that the states exhibiting the highest and lowest REEs for a given value of the nonlocality and demonstrating that mixed states can be more entangled than pure states if the fixed nonlocality is less than 0.8169.

II. DEFINITIONS

Hereafter, we study general two-qubit density matrices ρ , which can be expressed in the standard Bloch representation as

$$\rho = \frac{1}{4}(I \otimes I + \vec{x} \cdot \vec{\sigma} \otimes I + I \otimes \vec{y} \cdot \vec{\sigma} + \sum_{n,m=1}^3 T_{nm} \sigma_n \otimes \sigma_m), \quad (1)$$

where $\vec{\sigma} = [\sigma_1, \sigma_2, \sigma_3]$ and the correlation matrix $T_{ij} = \text{Tr}[\rho(\sigma_i \otimes \sigma_j)]$ are given in terms of the three Pauli matrices, and $x_i = \text{Tr}[\rho(\sigma_i \otimes I)]$ ($y_i = \text{Tr}[\rho(I \otimes \sigma_i)]$) are the elements of the Bloch vector \vec{x} (\vec{y}) of the first (second) subsystem. Expressing the two-qubit density matrix by Eq. (1) is very convenient since it allows a direct application of an effective criterion for the nonlocality.

A. Nonlocality measure

The two-qubit Bell inequality in the form derived by Clauser, Horne, Shimony and Holt (CHSH) [2] can be formulated as

$$|\text{Tr}(\rho \mathcal{B}_{\text{CHSH}})| \leq 2, \quad (2)$$

where the Bell-CHSH operator is $\mathcal{B}_{\text{CHSH}}$ is given by

$$\mathcal{B}_{\text{CHSH}} = \vec{a} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b}') \cdot \vec{\sigma} + \vec{a}' \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b}') \cdot \vec{\sigma}, \quad (3)$$

and its expected value is maximized over real-valued three-dimensional unit vectors \vec{a} , \vec{a}' , \vec{b} , and \vec{b}' . According to the Horodecki theorem, the maximum expected value of the Bell-CHSH operator for a given state ρ reads as [21, 22]:

$$\max_{\mathcal{B}_{\text{CHSH}}} \text{Tr}(\rho \mathcal{B}_{\text{CHSH}}) = 2\sqrt{M(\rho)} \quad (4)$$

given in terms of the parameter

$$M(\rho) = \max_{j < k} \{h_j + h_k\} \leq 2, \quad (5)$$

where h_j ($j = 1, 2, 3$) are the eigenvalues of the real symmetric matrix $U = T^T T$ constructed from the correlation matrix T and its transpose T^T . Hence, the condition for violating the Bell-CHSH inequality is $M(\rho) > 1$ [21, 22]. For convenience, we refer to *nonlocality* as the violation of the Bell-CHSH inequality.

To quantify a degree of the nonlocality, one can directly use $M(\rho)$ or $2\sqrt{M(\rho)}$ (see, e.g., Refs. [23, 24]), or more naturally $\max[0, M(\rho) - 1]$ (see, e.g., Ref. [18]). However, we decided to use another function of $M(\rho)$, denoted by $B(\rho)$, which for two-qubit pure states is equal to the concurrence and negativity. This measure can be given as [16]:

$$B(\rho) \equiv \sqrt{\max[0, M(\rho) - 1]}. \quad (6)$$

We see that $B(\rho) = 0$ if a given state ρ satisfies the Bell-CHSH inequality, given by Eq. (2), and $B(\rho) = 1$ if the inequality is maximally violated. The value of $B > 0$ increases with M , thus, it can be used to quantify the BIV. We refer to this BIV degree as *nonlocality* measure.

B. Entanglement measures

Now, we recall some definitions of a few selected measures of entanglement applicable for two-qubit entangled states.

In our considerations, the most important entanglement measure is the REE defined as $E_R(\rho) = \min_{\sigma \in \mathcal{D}} S(\rho||\sigma)$, which is the relative entropy $S(\rho||\sigma) = \text{Tr}(\rho \log_2 \rho - \rho \log_2 \sigma)$ minimized over a set \mathcal{D} of separable states σ [7, 25]. This measure is a quantum counterpart of the Kullback-Leibler divergence quantifying the difference between two classical probability distributions. Evidently, the REE is limited, by definition, to distinguishing a density matrix ρ from the closest separable state (CSS) σ only. Note that the REE is not a true metric, since it is not symmetric and does not fulfill the triangle inequality. However, the REE has a desirable property of a good entanglement measure that, for pure states, it reduces to the von Neumann entropy of one of the subsystems.

Unfortunately, as discussed in Refs. [26–29], it is very unlikely to find an analytical compact formula for the REE of a general two-qubit mixed state, which would correspond to finding its closest separable state (CSS). Numerical procedures for calculating the two-qubit REE correspond usually to an optimization problem over 79 or more real parameters [17, 25, 30]. On the other hand, there is a compact-form solution of the inverse problem: If a CSS is known then all the entangled states (having the same CSS) can be given analytically not only for two qubits [27, 28] but even for arbitrary multipartite states of any dimensions [31].

The second measure studied here is the negativity [13, 32, 33], defined as $N(\rho) = \max\{0, -2\mu_{\min}\}$, where $\mu_{\min} = \min \text{eig}(\rho^\Gamma)$ and Γ denotes partial transpose. The negativity is related to the logarithmic negativity, $\log_2[N(\rho) + 1]$, which is a measure of the entanglement cost under the PPT operations [8, 34]. These two related measures reach unity for the Bell states and vanish for separable states, however, for clarity of our further presentation, we will use only the negativity.

The last entanglement measure applied in this paper is the concurrence introduced by Wootters [11] as $C(\rho) = \max\{0, 2\lambda_{\max} - \sum_j \lambda_j\}$, where $\lambda_j^2 = \text{eig}[\rho(\sigma_2 \otimes \sigma_2)\rho^*(\rho_2 \otimes \sigma_2)]_j$ and $\lambda_{\max} = \max_j \lambda_j$. This measure is directly related to the entanglement of formation, $E_F(\rho)$ [12]. However, for

the same reason as in the case of the negativity we use the concurrence instead of $E_F(\rho)$.

III. ANALYTICAL COMPARISON OF ENTANGLEMENT AND NONLOCALITY FOR SPECIAL STATES

In Fig. 1, we presented several curves corresponding, in particular, to the Horodecki states, Bell-diagonal states and pure states. The REE for these states can be calculated analytically so let us first discuss and compare them to demonstrate the main point of our paper.

A. Pure states

We can simply relate all the above-mentioned entanglement and nonlocality measures in a special case of an arbitrary two-qubit pure states $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$ (with the normalization condition $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$) as

$$B(|\psi\rangle) = C(|\psi\rangle) = N(|\psi\rangle) = 2|ad - bc|. \quad (7)$$

Moreover, in this special case B , N and C are simply related to the REE and von Neumann's entropy S as

$$\mathcal{W}(B) = E_R(|\psi\rangle) = S(\rho_i), \quad (8)$$

where $\mathcal{W}(B) \equiv h(\frac{1}{2}[1 + \sqrt{1 - B^2}])$ is the Wootters function [11] given in terms of the binary entropy $h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x)$, and $\rho_i = \text{Tr}_{3-i} \rho$ is the reduced density matrix of the i th qubit.

B. Horodecki states

Let us also analyze a mixture of a Bell state, say $|\psi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$, and vacuum state, i.e.,

$$\rho^{(H)}(p) = \rho^{(A)}(1/2, p) = p|\psi^+\rangle\langle\psi^+| + (1-p)|00\rangle\langle 00|, \quad (9)$$

which is referred to as the Horodecki state. By applying Eq. (5), we find that $M(\rho^{(H)}) = p^2 + \max[p^2, (1 - 2p)^2]$. Thus, the nonlocality B is given by

$$B(\rho^{(H)}) = \sqrt{\max(0, 2p^2 - 1)}. \quad (10)$$

On the other hand, the entanglement measures are the following: the concurrence is $C(\rho^{(H)}) = p$, the negativity is $N(\rho^{(H)}) = \sqrt{(1-p)^2 + p^2} - (1-p)$, and the REE reads as

$$\begin{aligned} E_R(\rho^{(H)}) &= 2h(1 - p/2) - h(p) - p \\ &= (p - 2) \log_2(1 - p/2) + (1 - p) \log_2(1 - p). \end{aligned} \quad (11)$$

It is seen that the Horodecki state is entangled for $0 < p \leq 1$, while it is violating the Bell-CHSH inequality only for $1/\sqrt{2} < p \leq 1$. By comparing the REEs for a given nonlocality for the Horodecki and pure states we find that

$$\begin{aligned} E_R^{(H)}(B) &> E_R^{(P)}(B) \quad \text{for } 0 < B < B_6, \\ E_R^{(H)}(B) &< E_R^{(P)}(B) \quad \text{for } B_6 < B < 1, \end{aligned} \quad (12)$$

where $B_6 \equiv B(\rho_6) = 0.5856$ and $E_R^{(H)}(B_6) = E_R^{(P)}(B_6) = 0.4520$ [see Tab. I and Fig. 3(b)]. This means that mixed states can be more entangled than pure states at least for $B < B(\rho_6)$. Fig. 1(c) shows that this property holds up to $B < B(\rho_5) = 0.8169$ but for other mixed states, which is demonstrated in Sec. V. Here, $E_R^{(H)}$ as a function of B is explicitly given by Eq. (11) for $p = \sqrt{(1 + B^2)/2} \geq 1/\sqrt{2}$.

Analogous comparison of the REEs for a given negativity N for the Horodecki and pure states [see Fig. 1(b)] shows that [17]:

$$\begin{aligned} E_R^{(H)}(N) &> E_R^{(P)}(N) \quad \text{for } 0 < N < N_1, \\ E_R^{(H)}(N) &< E_R^{(P)}(N) \quad \text{for } N_1 < N < 1, \end{aligned} \quad (13)$$

where $N_1 \equiv N(\rho_1) = 0.3770$ and $E_R^{(H)}(N_1) = E_R^{(P)}(N_1) = 0.2279$ [see Tab. I and Fig. 3(a)]. Note that $E_R^{(H)}$ as a function of N can be given explicitly by Eq. (11) as $p = \sqrt{2N(1 + N)} - N$.

It is convenient to introduce a parameter $\Delta E_R(X)$, which is the maximal difference in the REE between a given mixed state ρ and some pure state $\rho^{(P)} = |\psi\rangle\langle\psi|$ having the same value of either the nonlocality ($X = B$) or negativity ($X = N$), i.e.,

$$\begin{aligned} \Delta E_R(X') &= \max_X \{E_R[\rho(X)] - E_R[\rho^{(P)}(X)]\} \\ &= E_R[\rho(X')] - E_R[\rho^{(P)}(X')], \end{aligned} \quad (14)$$

where X' is the optimal value of X . For the Horodecki state, we observe that this maximal difference for the nonlocality is equal to $\Delta E_R^{(H)}(B') = 0.2949$, which occurs for $B' = 0$, while for the negativity is only $\Delta E_R^{(H)}(N') = 0.0391$, which is for $N' = 0.1540$.

C. Bell-diagonal states

Finally, let us also analyze the Bell-diagonal states (labeled by D), which are defined by

$$\rho^{(D)} = \sum_{i=1}^4 \lambda_i |\beta_i\rangle\langle\beta_i|, \quad (15)$$

where $|\beta_i\rangle$ are the Bell states and $0 < \lambda_j < 1$ such that $\sum_j \lambda_j = 1$ with the largest eigenvalue $\max_j \lambda_j \equiv (1 + N)/2 \geq 1/2$. The nonlocality of the Bell-diagonal state $\rho^{(D)}$ is given by [16]:

$$B(\rho^{(D)}) = \sqrt{\max\{0, 2 \max_{(i,j,k)} [(\lambda_i - \lambda_j)^2 + (\lambda_k - \lambda_4)^2] - 1\}}, \quad (16)$$

where subscripts (i, j, k) correspond to the cyclic permutations of $(1, 2, 3)$. By contrast, the negativity and concurrence are the same and simply given by $N(\rho^{(D)}) = C(\rho^{(D)}) = N$. The REE versus the negativity (and, thus, also the concurrence) reads as

$$E(\rho^{(D)}) = 1 - h\left(\frac{1 + N}{2}\right) \quad (17)$$

TABLE I. Nonlocality and entanglement measures of the amplitude-damped states $\rho_n = \rho^{(A)}(\alpha, p)$ (for $n = 1, \dots, 6$), given by Eq. (25), corresponding to the characteristic points marked in Fig. 1.

State	α	p	C	N	E_R	B
ρ_1	0.0369	1.0000	0.3770	0.3770	0.2279	0.3770
ρ_2	0.0751	1.0000	0.5271	0.5271	0.3847	0.5271
ρ_3	0.2198	0.8536	0.7070	0.5756	0.4039	0.0000
ρ_4	0.3510	0.9565	0.9130	0.8706	0.7445	0.8169
ρ_5	0.2116	1.0000	0.8169	0.8169	0.7445	0.8169
ρ_6	0.0947	1.0000	0.5856	0.5856	0.4520	0.5856

as given in terms of the binary entropy h . If $\max_j \lambda_j \leq 1/2$ then the state is separable $E(\rho^{(N)}) = 0$.

It is evident that the nonlocality of the Bell-diagonal states depends on all probabilities λ_i , while the entanglement measures depend solely on the largest value $\max_i \lambda_i > 1/2$. Nevertheless, in some special cases of these states, the entanglement and nonlocality measures can be equal. For example, when only two probabilities λ_i corresponding to $|\psi^\pm\rangle$ are nonzero, the Bell-diagonal state $\rho^{(D)}$ reduces to

$$\rho^{(D2)} = p|\psi^+\rangle\langle\psi^+| + (1-p)|\psi^-\rangle\langle\psi^-|, \quad (18)$$

which is studied in a physical context in Sec. IV. The nonlocality for this rank-2 state is simply given by

$$B(\rho^{(D2)}) = |2p - 1| \quad (19)$$

implying that

$$E(\rho^{(D2)}) = 1 - h\left(\frac{1+B}{2}\right), \quad (20)$$

which corresponds to Eq. (17).

It is seen in Figs. 1(b,c) (see also Sec. V for a partial proof) that the lower bounds of the REE vs negativity and the REE vs nonlocality correspond to the Bell-diagonal state $\rho^{(D)}$, which satisfy the extremal KKT conditions as we show in Sec. V. Their physical context is discussed below.

IV. MANIPULATING ENTANGLEMENT AND NONLOCALITY VIA DAMPING CHANNELS

In Fig. 1, we have presented the entanglement and nonlocality measures for a million randomly-generated two-qubit states using the Monte Carlo simulation. It is seen that pure states are maximally entangled in terms of the REE for an arbitrary concurrence as shown in Fig. 1(a). However, pure states are not always maximally entangled for the cases shown in Figs. 1(a,b). Namely, the red regions correspond to mixed states having the REE higher than that for pure states for given negativity [Fig. 1(b)] and nonlocality [Fig. 1(c)].

This is a counterintuitive result, so to have a deeper physical meaning of the states corresponding to the red regions in Fig. 1, let us analyze the loss of entanglement between

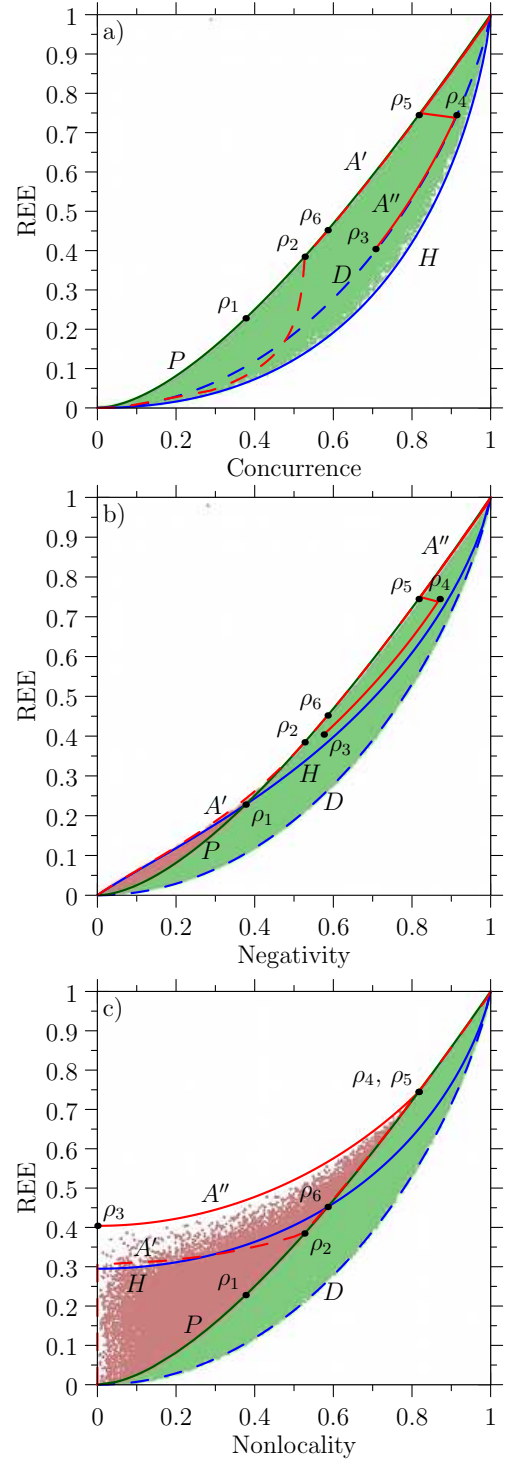


FIG. 1. (Color online) Monte Carlo simulations of about 10^6 two-qubit states ρ for the relative entropy of entanglement, $E_R(\rho)$, versus: (a) concurrence $C(\rho)$, (b) negativity $N(\rho)$, and (c) nonlocality $B(\rho)$ corresponding to the Bell-CHSH inequality violation. Red regions correspond to mixed states more entangled than pure states in terms of the $E_R(\rho)$. Key: P – pure states, D – the Bell-diagonal states ($\alpha = 0.5$), A' (A'') – the MEMS, which are the amplitude-damped states optimized for the case b (c), H – the Horodecki states, and the coordinates of points ρ_n (where $n = 1, \dots, 6$) are given in Tab. I.

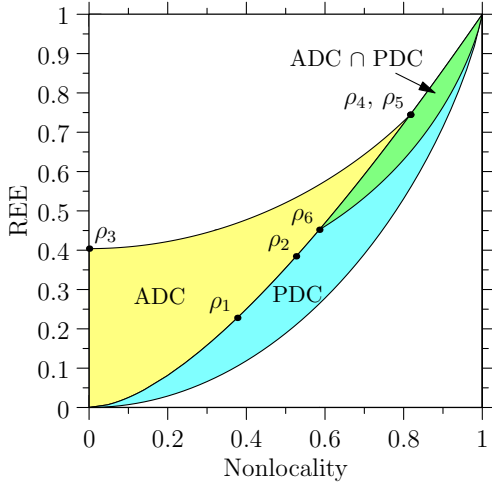


FIG. 2. (Color online) Ranges of the relative entropy of entanglement for a given nonlocality for the two-qubit mixed states generated from pure states by the amplitude damping channel, given by Eq. (25) (yellow and green areas) and the phase damping channel, given by Eq. (32) (blue and green areas).

two qubits initially in a pure state. In particular, by taking one of the Bell states $|\psi^\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$ or $|\phi^\pm\rangle = (I \otimes \sigma_1)|\psi^\pm\rangle$ as an initial state, one can achieve any degree of entanglement between the two qubits by coupling them to their environment(s). Note, however, that by coupling qubits to separated and uncorrelated environments, we can only decrease the entanglement, since any local operation cannot increase it. Damping can occur in various ways, but we focus on states generated from pure states by three prototype damping models (channels), for which the ranges of the REE for a given value of the nonlocality is shown in Fig. 2. We show in detail that these damping channels provide us with the mixed states with extreme values of the REE for a fixed value of another entanglement or nonlocality measures.

In this section we analyze the effect of the prototype damping channels on pure states of the form

$$|\psi_\alpha\rangle = \sqrt{\alpha}|01\rangle + \sqrt{1-\alpha}|10\rangle, \quad (21)$$

where $0 \leq \alpha \leq 1$. When analyzing the entanglement measures, any pure two-qubit state, as given above Eq. (7), can be equivalently expressed by means of the Schmidt decomposition, in the form given by Eq. (21). Although damping of these pure states can lead to inequivalent states, for simplicity, we confine our analysis only to the input states $|\psi_\alpha\rangle$.

A convenient description of damping can be given in terms of the Kraus operators E_i (specified below). Two-side damping of the state $\rho_{\text{in}}(\alpha) = |\psi_\alpha\rangle\langle\psi_\alpha|$ leads to the following output state

$$\rho(\alpha, q_1, q_2) = \sum_{i,j} [E_i(q_1) \otimes E_j(q_2)] \rho_{\text{in}}(\alpha) [E_i^\dagger(q_1) \otimes E_j^\dagger(q_2)], \quad (22)$$

where the Kraus operators satisfy the normalization relation $\sum_i E_i^\dagger(q) E_i(q) = I$. In the special case of the one-side

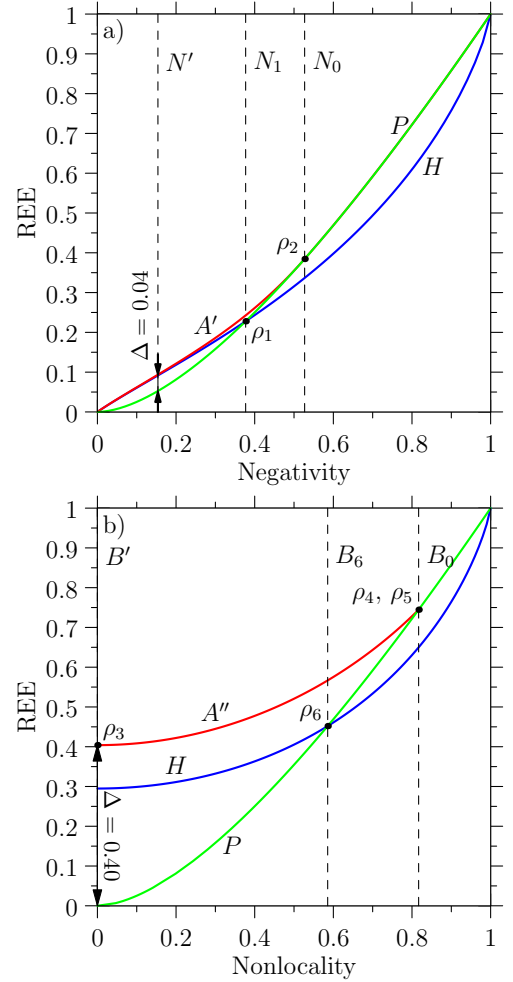


FIG. 3. (Color online) Ranges of the relative entropy of entanglement for given values of (a) negativity and (b) nonlocality. It is seen that the maximal difference in the REE between the optimal states and pure states is equal to (a) $\Delta = \Delta E_R(N') = 0.0391$ at the negativity $N' = 0.154$ and (b) $\Delta = \Delta E_R(B') = 0.404$ at the nonlocality $B' = 0$. Pure states become more entangled than the Horodecki states $\rho^{(H)}(p) = \rho^{(A)}(\frac{1}{2}, p)$ for (a) $N > N(\rho_1) = 0.377$ and (b) $B > B(\rho_6) = 0.586$. While pure states become optimal for (a) $N > N_0 \equiv N(\rho_2) = 0.527$ and (b) $B > B_0 \equiv B(\rho_4) = B(\rho_5) = 0.817$. The states ρ_n (for $n = 1, \dots, 6$) are specified in Tab. I.

damping (say $q_2 = 0$), Eq. (22) reduces to

$$\rho(\alpha, q_1) = \sum_i [E_i(q_1) \otimes I] \rho_{\text{in}}(\alpha) [E_i^\dagger(q_1) \otimes I]. \quad (23)$$

A. Amplitude-damping channel

The Kraus operators for the single-qubit amplitude-damping channel (ADC) are the following [3]:

$$E_0(q_i) = |0\rangle\langle 0| + \sqrt{p_i}|1\rangle\langle 1|, \quad E_1(q_i) = \sqrt{q_i}|0\rangle\langle 1|, \quad (24)$$

where $q_i \equiv 1 - p_i$ is the amplitude-damping coefficient. One can find that the pure state $|\psi_\alpha\rangle$ after passing through the ADC

is changed into the following mixed state

$$\rho^{(\text{adc})}(\alpha, q_1, q_2) = p|\psi_{\alpha'}\rangle\langle\psi_{\alpha'}| + q|00\rangle\langle 00| \equiv \rho^{(A)}(\alpha', p), \quad (25)$$

where the effective damping constant reads as $q \equiv 1 - p = \alpha q_2 + (1 - \alpha)q_1$ and $|\psi_{\alpha'}\rangle$ is given by Eq. (21) but for $\alpha' = \alpha p_2 / [\alpha p_2 + (1 - \alpha)p_1]$, which can take values from 0 to α , where $\alpha' = \alpha$ is achieved for the symmetric two-side ADC, i.e., when $q_1 = q_2$. The state given by Eq. (25) is sometimes referred to as the generalized Horodecki state (see, e.g., Refs. [17, 28]). Hereafter, we refer to the discussed states $\rho^{(A)}(\alpha', p)$ as the amplitude-damped states. The range of the REE for a given nonlocality for the ADC state, given by Eq. (25), is shown in Fig. 2.

In the special case, when $\alpha p_2 = (1 - \alpha)p_1$, which implies $\alpha' = 1/2$, the ADC reduces to the Horodecki state (see e.g. Ref. [35]), i.e.,

$$\rho^{(H)}(p) = \rho^{(A)}(\frac{1}{2}, p) = p|\psi^+\rangle\langle\psi^+| + q|00\rangle\langle 00|, \quad (26)$$

as given by Eq. (9). These states can be obtained from the initial Bell state $|\psi^+\rangle$ subjected to the symmetric two-side ADC, but they can be also obtained by asymmetric two-side ADC (or even the one-side ADC) of the initially non-maximally entangled pure state $|\psi_{\alpha}\rangle$.

We find that the nonlocality of the ADC state for any α is given by

$$B(\rho^{(A)}) = \sqrt{\max\{0, \max[x, (1 - 2p)^2] + x - 1\}}, \quad (27)$$

where $x = 4(1 - \alpha')\alpha'p^2$. By comparison, the negativity reads as

$$N(\rho^{(A)}) = \sqrt{(1 - p)^2 + x} - (1 - p), \quad (28)$$

and the concurrence is $C(\rho^{(A)}) = \sqrt{x}$. By contrast to these simple formulas, there is no analytical formula for the REE for $\rho^{(A)}$ for arbitrary α and p , except some special cases. For example, the REE can be calculated analytically, according to Eq. (11), for the Horodecki states, given by Eq. (26).

Our numerical calculations shown in Fig. 1(c) indicate that the Bell-diagonal states are likely to be the lower bound for the REE vs nonlocality. Thus, let us analyze whether the ADC states can be diagonal in the Bell basis. By denoting the Bell states as follows $|\beta_1\rangle = |\psi^-\rangle$, $|\beta_2\rangle = |\psi^+\rangle$, $|\beta_3\rangle = |\phi^-\rangle$, and $|\beta_4\rangle = |\phi^+\rangle$, we find that the ADC state can be given in the Bell basis as:

$$\rho^{(\text{adc})}(\alpha, q_1, q_2) = r_-|\beta_1\rangle\langle\beta_1| + r_+|\beta_2\rangle\langle\beta_2| + r|\beta_3\rangle\langle\beta_3| + r|\beta_4\rangle\langle\beta_4| + (t|\beta_2\rangle\langle\beta_1| + r|\beta_4\rangle\langle\beta_3| + \text{h.c.}), \quad (29)$$

where $t = \alpha(1 - q_2) + r - \frac{1}{2}$; $r_{\pm} = \frac{1}{2}[1 - 2r \pm C(\rho^{(A)})]$, and $r = \frac{1}{2}[(1 - \alpha)q_1 + \alpha q_2]$. So, this state is diagonal in the Bell basis only if $\alpha = 0$ and 1. Note that for $\alpha = 1/2$, one has $r_- = \frac{1}{4}(p_1 - p_2)^2$, which vanishes for $p_1 = p_2$, but another off-diagonal term $r = \frac{1}{4}(q_1 + q_2)$ vanishes only if there is no damping at all. This shows (as also confirmed numerically in Fig. 2) that the ADC states do not have the minimum of the REE for a given nonlocality except only two points for $B = 0$ and 1. By contrast, Figs. 1(c) and 2 show that the ADC states are likely to be the upper bound of the REE vs nonlocality. This observation is confirmed analytically in Sec. V.

B. Phase-damping channel

The Kraus operators for the single-qubit phase-damping channel (PDC) can be given by [3]:

$$E_0(q_i) = |0\rangle\langle 0| + \sqrt{p_i}|1\rangle\langle 1|, \quad E_1(q_i) = \sqrt{q_i}|1\rangle\langle 1|, \quad (30)$$

where $q_i = 1 - p_i$ is the phase-damping coefficient. Thus, one can find that the pure state $|\psi_{\alpha}\rangle$ after being transmitted through the PDC is changed into the following mixed state

$$\rho^{(\text{pdc})}(\alpha, q_1, q_2) = \alpha|01\rangle\langle 01| + (1 - \alpha)|10\rangle\langle 10| + y(|01\rangle\langle 10| + |10\rangle\langle 01|), \quad (31)$$

where $y = \sqrt{\alpha(1 - \alpha)p_1p_2}$. This state can be also given as

$$\rho^{(\text{pdc})}(\alpha, q_1, q_2) = p''|\psi_{\alpha''}\rangle\langle\psi_{\alpha''}| + q''|01\rangle\langle 01|, \quad (32)$$

where the effective damping constant can be defined as $q'' \equiv 1 - p'' = \alpha(1 - p_1p_2)$ and the pure state $|\psi_{\alpha''}\rangle$ is given by Eq. (21) but for $\alpha'' = \alpha p_1p_2/p''$, which takes the values $0 \leq \alpha'' \leq \alpha$. Note that if $\alpha = p_1p_2/(q_1 + q_2 - q_1q_2)$ then $\alpha'' = \alpha$.

We find that the nonlocality, negativity and concurrence for the PDC state are equal to each other and are given by

$$B(\rho^{(\text{pdc})}) = N(\rho^{(\text{pdc})}) = C(\rho^{(\text{pdc})}) = 2y. \quad (33)$$

The range of the REE for a given nonlocality for the PDC state, given by Eq. (32), is shown in Fig. 2. Note that it is unlikely that there is analytical formula for the REE for the PDC states for arbitrary parameters α , q_1 , and q_2 . However, the REE can be found in some special cases. For example, if $\alpha = [1 + p_1p_2]^{-1} \equiv \alpha'$ then Eq. (32) reduces to

$$\rho^{(\text{pdc})}(\alpha', q_1, q_2) \equiv \rho^{(V)} = 2(1 - \alpha')|\psi^+\rangle\langle\psi^+| + (2\alpha' - 1)|01\rangle\langle 01|, \quad (34)$$

which means that $|\psi_{\alpha'}'\rangle$ becomes the Bell state $|\psi^+\rangle$. For this state, one finds that

$$B' \equiv B(\rho^{(V)}) = C(\rho^{(V)}) = N(\rho^{(V)}) = 2(1 - \alpha'). \quad (35)$$

The state $\rho^{(V)}$, the same as pure states, reaches the upper bound for the negativity versus concurrence [15]. The CSS for $\rho^{(V)}$ reads as $\sigma^{(V)} = (1 - B'/2)|01\rangle\langle 01| + (B'/2)|10\rangle\langle 10|$. Thus, the REE can simply be given by:

$$E_R(\rho^{(V)}) = h(\frac{1}{2}B') - h\{\frac{1}{2}[\sqrt{(1 - B')^2 + (B')^2} + 1]\}. \quad (36)$$

Now, we show that the minimum of the REE vs nonlocality can be reached by the PDC states. In the Bell basis, the PDC state is given by

$$\rho^{(\text{pdc})}(\alpha, q_1, q_2) = (\frac{1}{2} - y)|\beta_1\rangle\langle\beta_1| + (\frac{1}{2} + y)|\beta_2\rangle\langle\beta_2| + (\alpha - \frac{1}{2})(|\beta_1\rangle\langle\beta_2| + |\beta_2\rangle\langle\beta_1|), \quad (37)$$

which clearly becomes diagonal for initial Bell states (i.e., for $\alpha = 1/2$), given by Eq. (18) for $q \equiv 1 - p = 1/2 - y$ (see e.g. Ref. [35]). The REE for the state $\rho^{(D)}$ is given by Eq. (20). Hereafter, we consider only the case, when $\alpha = 1/2$ and use the shorthand notation $\rho^{(D)} \equiv \rho^{(D2)}$.

V. KARUSH-KUHN-TUCKER CONDITIONS FOR THE REE VS NONLOCALITY

In this section, we derive the KKT conditions, as a generalization of the method of Lagrange multipliers, in order to find the states with extremal values of the REE for a fixed value of the nonlocality.

Thus, let us consider the following Lagrange function:

$$\mathcal{L} = \text{Tr}(\rho \log \rho) - \text{Tr}(\rho \log \sigma) + l[\text{Tr}(\rho \mathcal{B}_{\text{CHSH}}) - \beta] - \text{Tr}(X\rho) + \lambda(\text{Tr}\rho - 1), \quad (38)$$

where l , λ , and X are Lagrange multipliers and $\beta = 2\sqrt{M(\rho)}$. For a small deviation of $\rho \rightarrow \rho + \Delta$, we have

$$\begin{aligned} \mathcal{L} &\rightarrow \mathcal{L} + \text{Tr}(\Delta \log \rho) - \text{Tr}(\Delta \log \sigma) \\ &\quad + \text{Tr}\left(\rho \int_0^\infty \frac{1}{\rho + z} \Delta \frac{1}{\rho + z} dz\right) \\ &\quad + l\text{Tr}(\Delta \mathcal{B}_{\text{CHSH}}) - \text{Tr}(\Delta X) + \lambda \text{Tr} \Delta \\ &\rightarrow \mathcal{L} + \text{Tr}[\Delta(\log \rho - \log \sigma + P \\ &\quad + l\mathcal{B}_{\text{CHSH}} - X + \lambda)], \end{aligned} \quad (39)$$

where P is a projector on the support space of ρ . Thus, the KKT conditions on the parameters l , λ , and X are the following:

$$\log \rho - \log \sigma + P + l\mathcal{B}_{\text{CHSH}} - X + \lambda = 0, \quad (40a)$$

$$X \geq 0, \quad \text{Tr}(X\rho) = 0. \quad (40b)$$

From the condition (40a), we obtain

$$\begin{aligned} 0 &= \text{Tr}(\rho \log \rho) - \text{Tr}(\rho \log \sigma) + \text{Tr}(\rho P) \\ &\quad + l\text{Tr}(\rho \mathcal{B}_{\text{CHSH}}) - \text{Tr}(\rho X) + \lambda \text{Tr} \rho \\ &= \gamma E_R(\rho) + 1 + l\beta + \lambda, \end{aligned} \quad (41)$$

where $\gamma = 1/\log_2 e$ and e is the base of the natural logarithm. Thus, $\lambda = -\gamma E_R(\rho) - 1 - l\beta$. Now, we can rewrite Eq. (40a) and obtain the simplified KKT conditions:

$$\begin{aligned} 0 &= \log \rho - \log \sigma + P + l\mathcal{B}_{\text{CHSH}} - X \\ &\quad - \gamma E_R(\rho) - 1 - l\beta, \end{aligned} \quad (42a)$$

$$X \geq 0, \quad \text{Tr}(X\rho) = 0. \quad (42b)$$

One can easily confirm that the condition

$$P[\log \rho - \log \sigma + l\mathcal{B}_{\text{CHSH}} - \gamma E_R(\rho) - l\beta]P = 0 \quad (43)$$

is a new KKT condition since $PX = 0$.

The boundary states are rank deficient. We search for them among the rank-2 states. We have a strong numerical evidence (see points for randomly-generated density matrices in Fig. 1) implying that the extreme two-qubit states can be found within the rank-2 class of mixed states. Thus, let us now consider the case where ρ is a rank-2 mixed state, i.e., $\rho = \lambda_1|e_1\rangle\langle e_1| + \lambda_2|e_2\rangle\langle e_2|$, where λ_i are non-zero eigenvalues of ρ , and $|e_i\rangle$ are the corresponding eigenstates. From Eq. (42b), we have

$$\langle e_1 | \log \sigma | e_2 \rangle = l \langle e_1 | \mathcal{B}_{\text{CHSH}} | e_2 \rangle, \quad (44a)$$

$$\begin{aligned} \gamma E_R(\rho) + l\beta &= \log \lambda_1 - \langle e_1 | \log \sigma | e_1 \rangle \\ &\quad + l \langle e_1 | \mathcal{B}_{\text{CHSH}} | e_1 \rangle, \end{aligned} \quad (44b)$$

from which l is determined. Then, there must exist X such that

$$\begin{aligned} X &= \log \rho - \log \sigma + P + l\mathcal{B}_{\text{CHSH}} \\ &\quad - [\gamma E_R(\rho) + 1 + l\beta] \geq 0, \end{aligned} \quad (45a)$$

$$\text{Tr}(X\rho) = 0. \quad (45b)$$

The KKT conditions, given by Eqs. (44a)–(45b), are the necessary conditions in searching for the boundary (extreme) states among rank-2 mixed states.

A. Lower bound of REE vs nonlocality

Here, we show the KKT conditions are satisfied by the Bell-diagonal states, given by Eq. (18), as obtained by the phase damping of the Bell states $|\psi^+\rangle$ or, equivalently, $|\psi^-\rangle$ assuming $p \leftrightarrow 1 - p$.

For these states the CSS is given

$$\sigma^{(D)} = \frac{1}{2}(|\psi^+\rangle\langle\psi^+| + |\psi^-\rangle\langle\psi^-|), \quad (46)$$

and the Bell-CHSH operator is

$$\begin{aligned} \mathcal{B}_{\text{CHSH}}^{(D)} &= \eta[-\sigma_3 \otimes \sigma_3 + (2p - 1)\sigma_1 \otimes \sigma_1] \\ &= 2\eta[p(|\psi^+\rangle\langle\psi^+| - |\phi^-\rangle\langle\phi^-|) \\ &\quad + (1 - p)(|\psi^-\rangle\langle\psi^-| - |\phi^+\rangle\langle\phi^+|)], \end{aligned} \quad (47)$$

where $\eta = 2/\sqrt{1 + (2p - 1)^2}$. So, by applying Eqs. (4) and (6), one can find the simple expression, given by Eq. (19), for the nonlocality.

Since it holds $\langle e_1 | \log \sigma^{(D)} | e_2 \rangle = \langle e_1 | \mathcal{B}_{\text{CHSH}}^{(D)} | e_2 \rangle = 0$, Eq. (44a) is satisfied for any l . From Eq. (44b), l is determined through

$$\log p + 1 + 2\eta pl = \gamma E_R^{(D)} + l\beta, \quad (48)$$

where $\beta = 2\sqrt{1 + (2p - 1)^2}$ and the REE is given by

$$E_R^{(D)} \equiv E_R(\rho^{(D)}) = 1 - h(p), \quad (49)$$

where $h(p)$ is the binary entropy defined below Eq. (8). Then, the KKT conditions are satisfied if

$$\begin{aligned} X &= -[\gamma E_R^{(D)} + 1 + l\beta + 2\eta l(1 - p)]|\phi^+\rangle\langle\phi^+| \\ &\quad - [\gamma E_R^{(D)} + 1 + l\beta + 2\eta lp]|\phi^-\rangle\langle\phi^-| \geq 0 \end{aligned} \quad (50)$$

for all values of p . Hence, the Bell-diagonal states can yield the extreme (in this case minimum) value of the REE for a given value of the nonlocality. This conclusion is confirmed by our Monte Carlo simulations (see Fig. 1).

B. Upper bound of REE vs nonlocality

Here, we show that the KKT conditions are also satisfied by the amplitude-damped states $\rho^{(A)}(\alpha, p)$, given by Eq. (25), for properly chosen parameters α and p . These MEMS having

the highest REE for a given negativity are shown by curves A'' in Figs. 1(c) and 3(b).

The support space of $\rho^{(A)}(\alpha, p)$ is given by the eigenvectors $|e_1\rangle = |00\rangle$ and $|e_2\rangle = |\psi_\alpha\rangle$. The corresponding CSS is given as [17]:

$$\sigma^{(A)}(\alpha, p) = R_1|00\rangle\langle 00| + R_4|11\rangle\langle 11| + \lambda_+|\lambda_+\rangle\langle \lambda_+| + \lambda_-|\lambda_-\rangle\langle \lambda_-|, \quad (51)$$

where

$$\lambda_\pm = \frac{1}{2} \left[R_2 + R_3 \pm \sqrt{(R_2 - R_3)^2 + 4R_1R_4} \right],$$

$$|\lambda_\pm\rangle = \Lambda_\pm \left[(\lambda_\pm - R_3)|01\rangle + \sqrt{R_1R_4}|10\rangle \right], \quad (52)$$

normalized by $\Lambda_\pm = [(\lambda_\pm - R_3)^2 + R_1R_4]^{-1/2}$. To calculate the CSS we have to compute

$$R_2 = \frac{1}{4} \left[1 + 3(1-p) + 2p\alpha - 4R_1 - \sqrt{\delta} \right],$$

$$R_4 = R_1 - 1 + p, \quad (53a)$$

$$R_3 = 1 - \sum_{i=1,2,4} R_i,$$

$$\delta = (4-3p)^2 - 4\alpha(1-\alpha)p^2 - 8R_1(2-p) + 16\sqrt{R_1(R_1-1+p)p^2\alpha(1-\alpha)}, \quad (53b)$$

where R_1 is obtained by solving

$$\alpha p = R_2 + 2R_4(R_2^2 - R_2R_3 + 2R_1R_4)/z^2 + 2R_4(R_2 - R_3)/(Lz), \quad (54)$$

where $z = \sqrt{(R_2 - R_3)^2 + 4R_1R_4}$ and $L = \log(R_2 + R_3 - z) - \log(R_2 + R_3 + z)$. The Bell-CHSH operator in this case reads as

$$\mathcal{B}_{\text{CHSH}}^{(A)} = \begin{cases} \eta_1 \left[(1-2p)\sigma_3^{\otimes 2} + 2p\sqrt{(1-\alpha)\alpha}\sigma_1^{\otimes 2} \right] & \text{if } 4p^2(1-\alpha)\alpha - (1-2p)^2 < 0, \\ \eta_2 p \sqrt{(1-\alpha)\alpha}(\sigma_1^{\otimes 2} + \sigma_2^{\otimes 2}) & \text{otherwise,} \end{cases} \quad (55)$$

where $\eta_1 = 2/\sqrt{(1-2p)^2 + 4p^2\alpha(1-\alpha)}$, $\eta_2 = 2/\sqrt{8p^2(1-\alpha)\alpha}$. Thus, by applying Eqs. (4) and (6), we find that the nonlocality is given by Eq. (27). Since we fix the value of β or equivalently $B \equiv B(\rho^{(A)})$, we can express p in terms of B and parameter α in the following way

$$\alpha = \begin{cases} \frac{1}{4p} \left(2p - \sqrt{2(2p^2 - B^2 - 1)} \right) & \text{if } 2\sqrt{2+2B^2} \leq 4p \leq 2 + \sqrt{2+2B^2}, \\ \frac{1}{2p} \left(p - \sqrt{5p^2 - 4p - B^2} \right) & \text{if } 2 + \sqrt{2+2B^2} < 4p \leq 4. \end{cases} \quad (56)$$

We can easily check by using Eqs. (55) and (51) that the condition, given by Eq. (44a), is always satisfied. Thus, the condition, given by Eq. (44b), is also satisfied. To check the remaining conditions, we need an explicit expression for the REE and multiplier l , which is equivalent to solving Eq. (54). This equation contains logarithms and can be easily solved only in

special cases as, e.g., the Horodecki states ($\alpha = 1/2$). Nevertheless, our numerical analysis reveals that for $\rho^{(A)}(\alpha, p)$, for which the REE reaches the largest value for a given value of nonlocality, Eq. (45b) is satisfied for the following coefficients of the amplitude-damped states:

$$p = \begin{cases} \frac{1}{4} (2 + \sqrt{2+2B^2}) & \text{if } B < B_0, \\ 1 & \text{if } B > B_0, \end{cases} \quad (57a)$$

$$1 \geq p \geq \frac{1}{4} \left(2 + \sqrt{2+2B_0^2} \right) \text{ if } B = B_0, \quad (57b)$$

$$\alpha = \frac{1}{2p} \left(p - \sqrt{5p^2 - 4p - B^2} \right), \quad (57c)$$

where $B_0 = 0.81686$ [see Fig. 3(b)].

Thus, by comparing the REEs for a given nonlocality for the optimal mixed states (denoted by subscript A'') and pure states, we can conclude that

$$E_R^{(A'')}(B) > E_R^{(P)}(B) \quad \text{for } 0 < B < B_0, \quad (58)$$

$$E_R^{(A'')}(B) < E_R^{(P)}(B) \quad \text{for } B_0 < B < 1,$$

where $B_0 = B(\rho_4) = B(\rho_5) = 0.81686$ and $E_R^{(A'')}(B_0) = E_R^{(P)}(B_0) = 0.7445$ [see Tab. I and Fig. 3(b)]. On the other hand, by comparing the REE for a given negativity for the optimal mixed states (denoted by subscript A') and pure states, it holds [17]:

$$E_R^{(A')}(N) > E_R^{(P)}(N) \quad \text{for } 0 < N < N_0, \quad (59)$$

$$E_R^{(A')}(N) < E_R^{(P)}(N) \quad \text{for } N_0 < N < 1,$$

where $N_0 = N(\rho_2) = 0.5271$ and $E_R^{(A')}(N_0) = E_R^{(P)}(N_0) = 0.3847$ [see Tab. I and Fig. 3(a)]. As a reminder, subscript A' (A'') corresponds to the amplitude-damped states $\rho^{(A')}$ ($\rho^{(A'')}$) optimized for the REE vs negativity (nonlocality). As shown in Fig. 1, the states $\rho^{(A')}$ and $\rho^{(A'')}$ are, in general, inequivalent. The maximal differences, as defined by Eq. (14), are equal to $\Delta E_R(N) = 0.2018$ for $N = 0.7071$, and $\Delta E_R(B) = 0.4040$ for $B = 0$. It is seen that ranges of mixed states, which are more entangled than pure states, are much smaller for the REE vs negativity in comparison to the REE vs nonlocality.

VI. CONCLUSIONS

We studied the relation between the relative entropy of entanglement E_R and the nonlocality measure B corresponding to a degree of the violation of the Bell-CHSH inequality in two-qubit systems. We found states of the extremal value of E_R for a given value of B . We showed that the obtained states satisfy the Karush-Kuhn-Tucker conditions, derived in Sec. V, as well as they provide a boundary for the REE values obtained by our Monte Carlo simulations presented in Fig. 1.

We demonstrated that mixed states can be more entangled in terms of E_R than pure states if the nonlocality $B \in (0, 0.82)$ and the maximal difference between these REEs is

$\Delta E_R = 0.4$ as shown in Fig. 3(b). As discussed in Ref. [17], E_R as a function of the negativity N can also exhibit this property but (i) the maximal difference ΔE_R is one-order smaller (i.e., $\Delta E_R = 0.039$) and (ii) mixed states are optimal for a shorter range of the negativity, i.e. $N \in (0, 0.53)$, as presented in Fig. 3(a). For appropriate comparison, we normalized B to be equal to N for any two-qubit pure state.

We showed that these maximally-entangled mixed states can be obtained from pure two-qubit entangled states by locally subjecting one or both qubits (of the entangled pair) to the amplitude-damping channel either. While the minimally-entangled states can be generated from pure states by subjecting one or both qubits to the phase-damping channel. We found that the amplitude-damped states (yellow and green areas in Fig. 2) are more entangled than the phase-damped states (blue and green areas) for a given nonlocality $B < 0.8169$ (corresponding to the nonlocality of the states ρ_4 and ρ_5 shown in Fig. 1 and Tab. I).

However, for values $B > 0.5856$ (point ρ_6) there exists a range of states, obtained either by the amplitude or phase damping, which have the same value of E_R for a given B (green area in Fig. 2). Moreover, we found that the upper bound on the REE of the phase-damped states (cyan and green areas in Fig. 2) for a given nonlocality is provided by pure states (curve P in Fig. 2). However, pure states have the high-

est REE only for $B > 0.8169$.

Thus, we found that for a large range of the nonlocality, mixed states can be more entangled than pure states, and, surprisingly, these mixed states can be obtained by the ordinary amplitude damping of pure states.

We believe that these results can stimulate further quest for practical protocols of quantum information processing for which mixed states are more effective than pure states.

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